Evaluated electron and positron-molecule scattering data for modelling particle transport in the energy range 0-10000 eV

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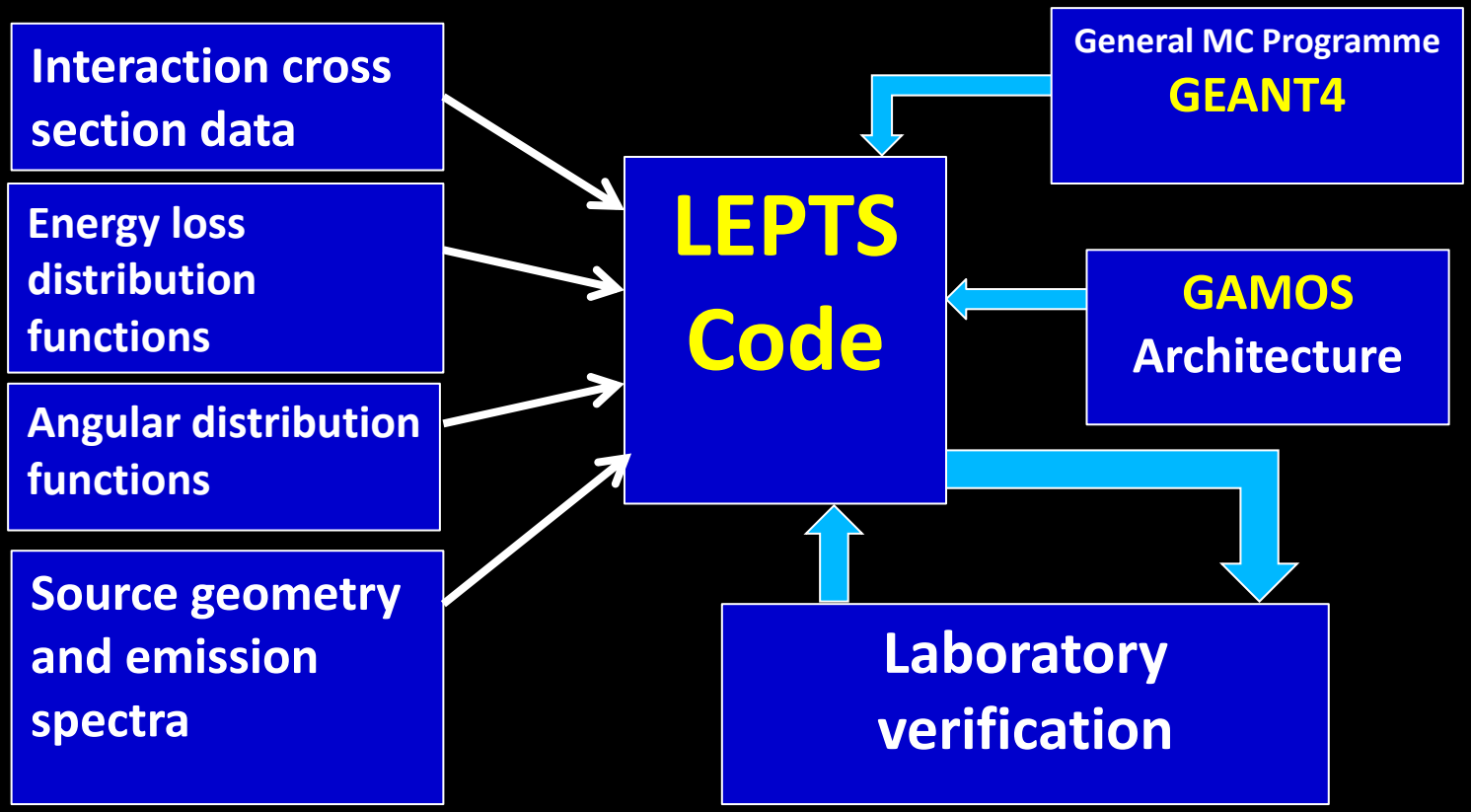
Modelling tools for molecular data validation

- High energy (E>10 keV) primary radiation (photons, electrons and ions):
  GEometry ANd Tracking4 (GEANT4)
- Low energy (E<10 keV) seconday particles (electrons, positrons and radicals):
  Low Energy Particle Track Simulation (LEPTS)

Modelling procedure to validate interaction data in molecular media



Input data

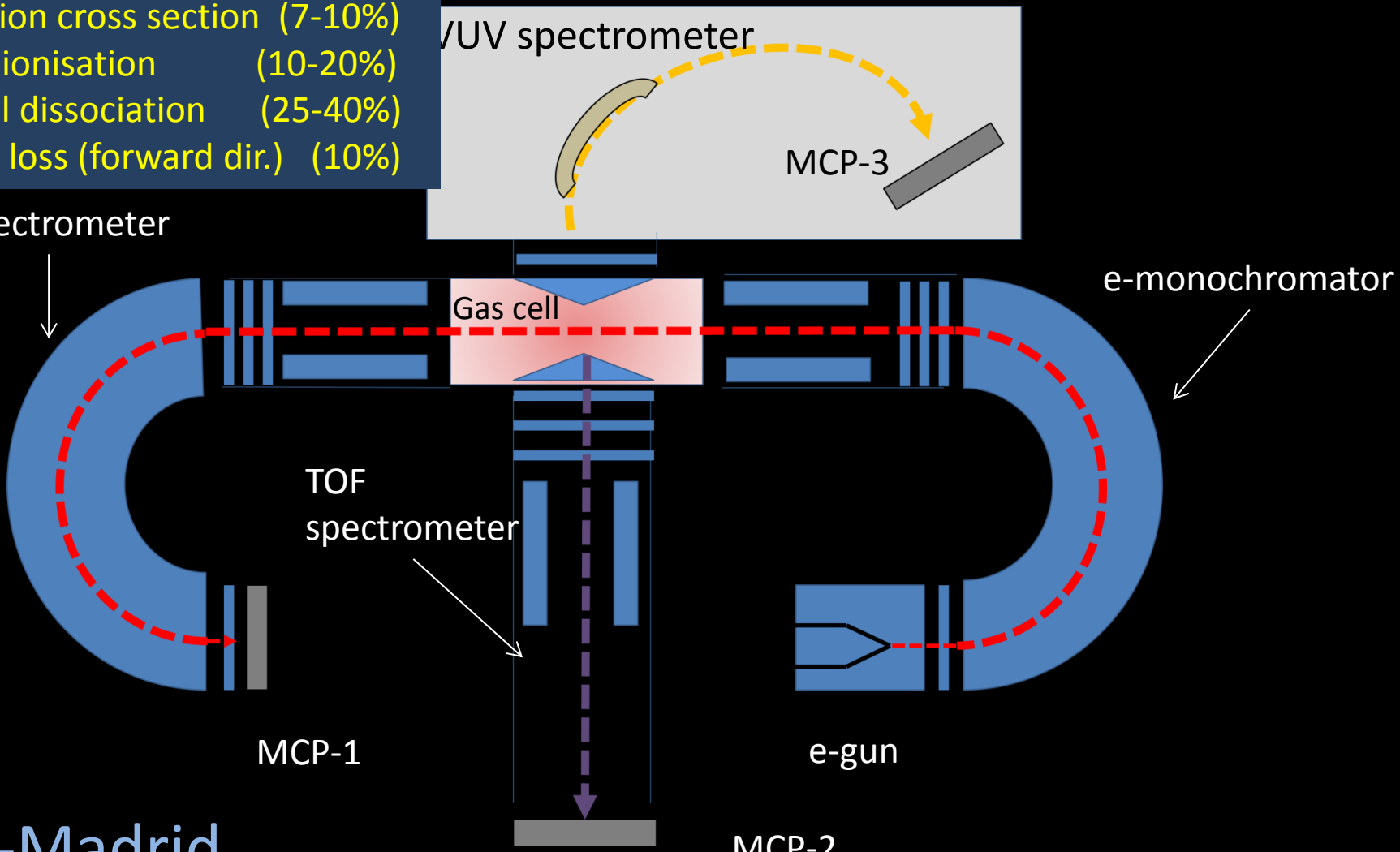
- High energy photons and ions:
  (Literature: Evaluated Data Bases)
- High energy (>10keV) electrons/positrons :
  (First Born approximation- Bethe surfaces)
- Low energy electron, positrons and radicals :
  (Evaluated theoretical and experimental data- EPEDAT)

Electron and positron evaluated data EPEDAT

- Experimental sources:
  - Electron and positron scattering with molecules: CSIC, Flinders University (FU), Universidade Nova de Lisboa (UNL), Sophia University (SU), Australian National University (ANU)
  - Electron transfer to molecules: CSIC, New University of Lisbon (UNL)
- Thoretical methods:
  - Electron and positron scattering with molecules: CSIC (IAM-SCAR), Open University (R-matrix), University of Innsbruck (Single-Centre Expansion)

Beam-gas experiments-1

Total cross cections	(5-7%)
Ionisation cross section	(7-10%)
Partial ionisation	(10-20%)
Neutral dissociation	(25-40%)
Energy loss (forward dir.)	(10%)

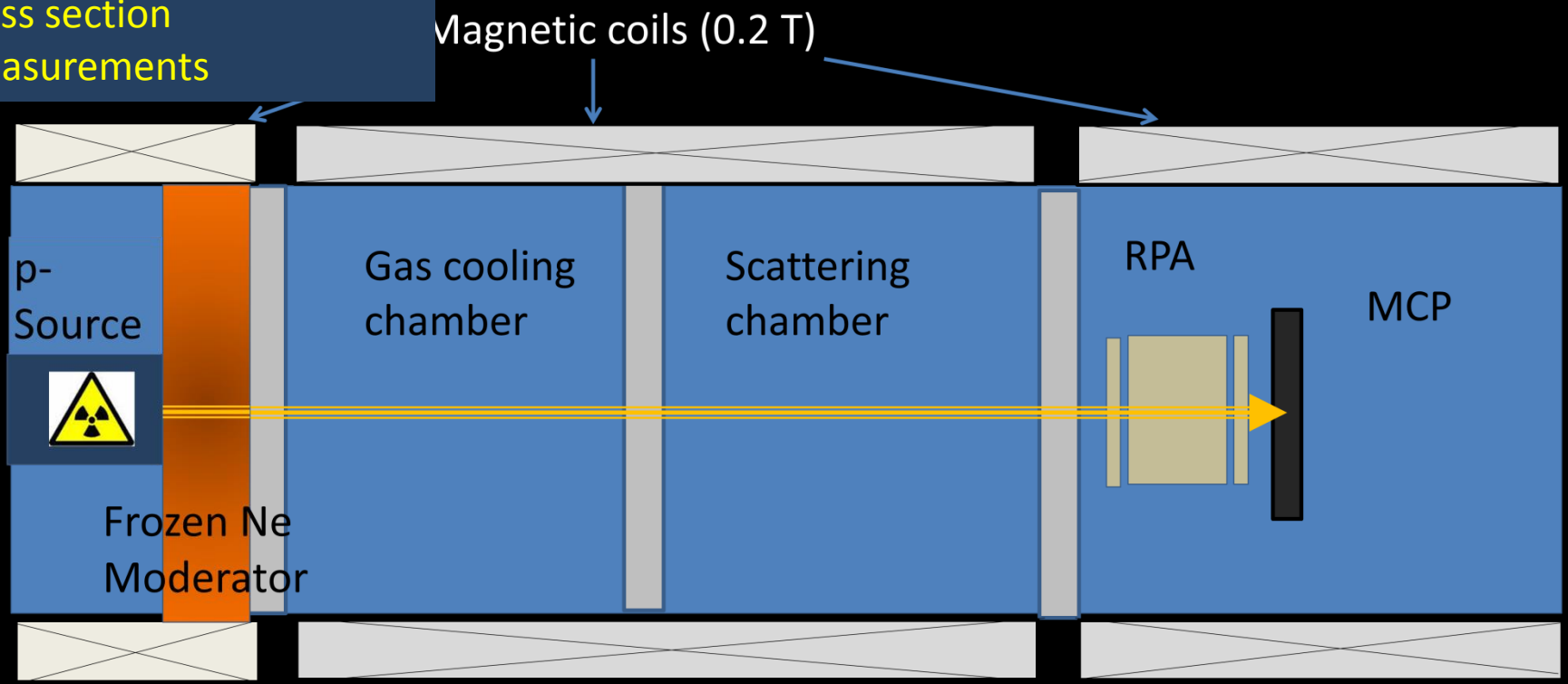


CSIC-Madrid

Beam-gas experiments-2

e/p magnetically confined beam

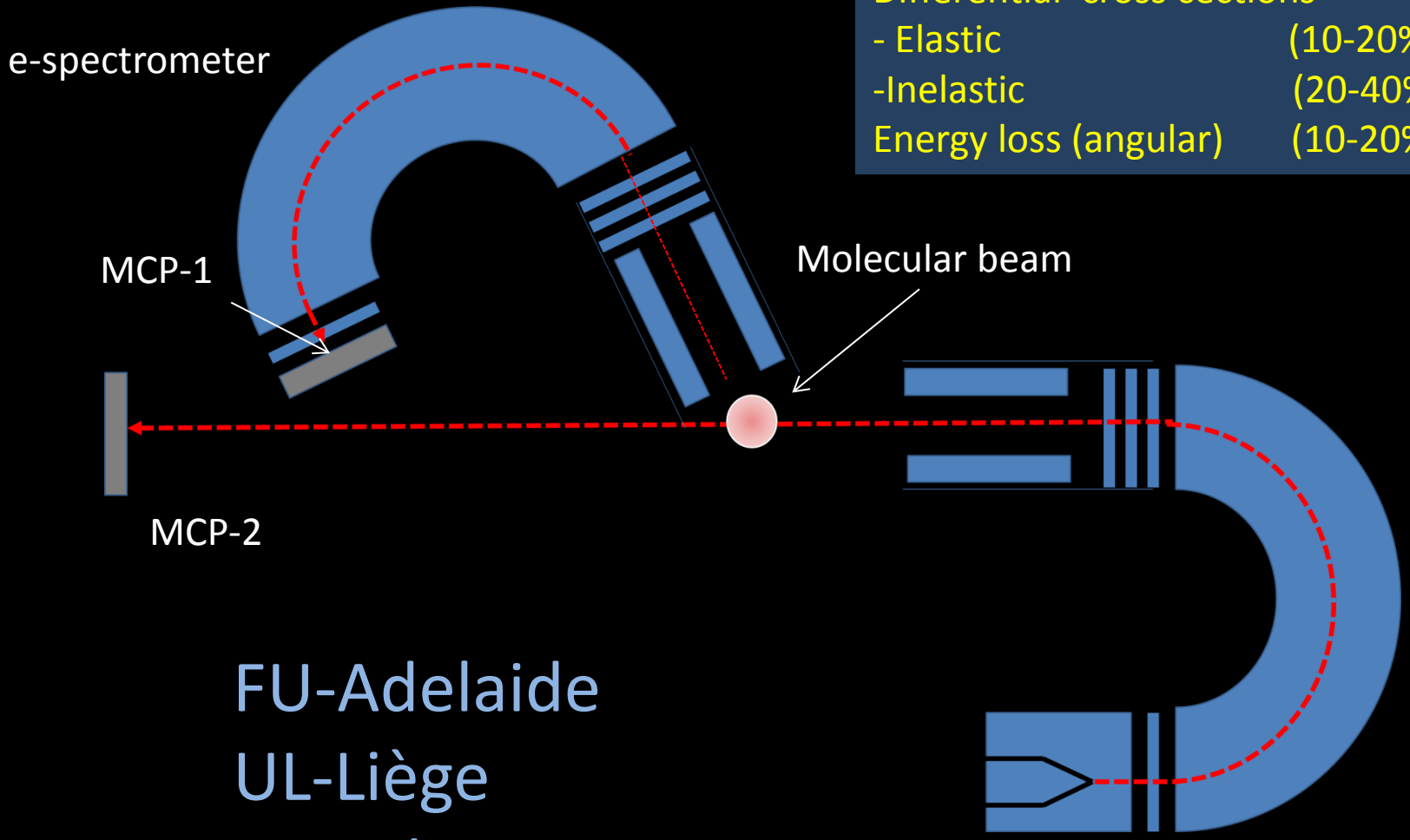
Differential and integral cross section measurements



ANU-Canberra (p) CSIC-Madrid (e)

Crossed-beam experiments-1

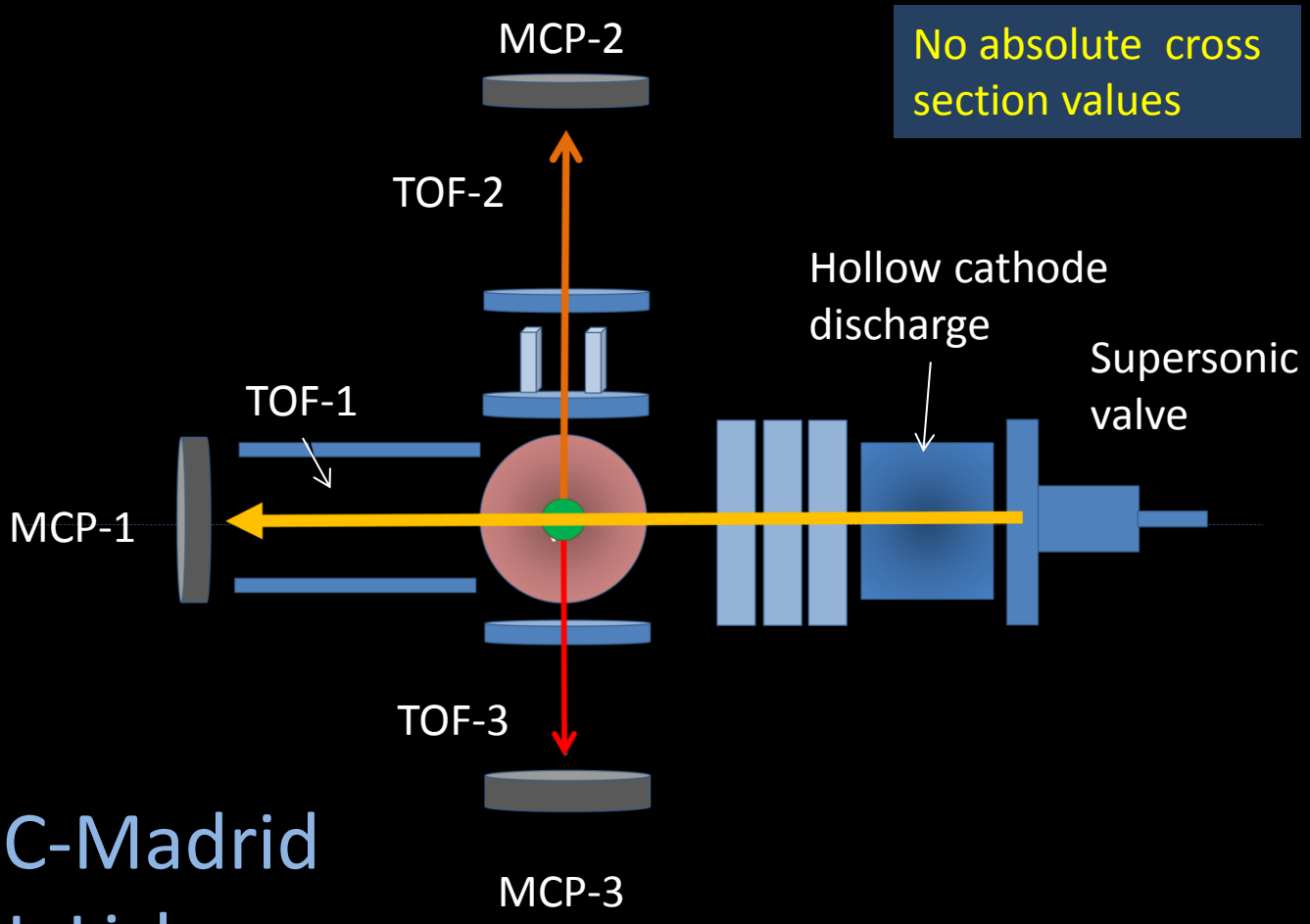
Differential cross cections
- Elastic (10-20%)
-Inelastic (20-40%)
Energy loss (angular) (10-20%)



FU-Adelaide
UL-Liège
SU-Tokyo

Crossed-beam experiments-2

electron transfer induced dissociation



No absolute cross section values

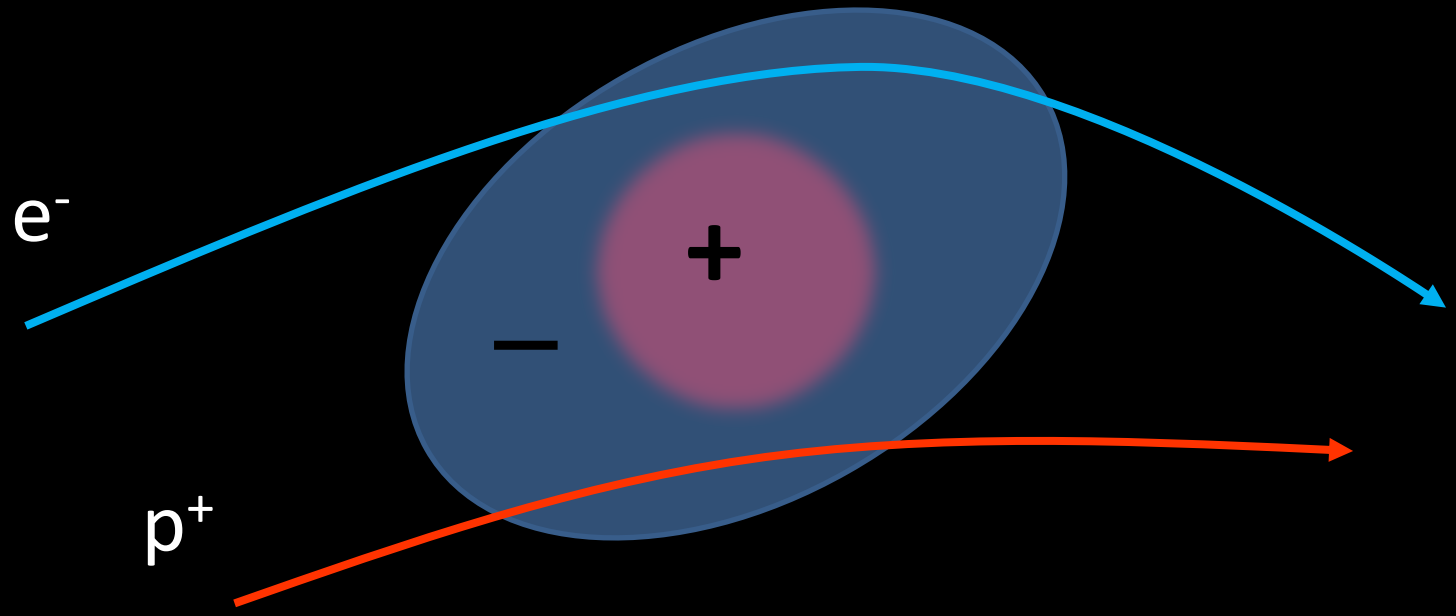
CSIC-Madrid
UNL-Lisbon

Calculations

Electron and positron scattering in molecular and condensed media

- **Atoms:** Model potential representation,
- **Molecules:**
  - **Independent atom model** (IAM), Aditivity rule (AR) with screening corrections (SCAR) and interference terms
  - **Additional dipole rotational excitations** (FBA)
- **Condensation effects:** Atomic and molecular clusters, liquids, solids (IAM-SCAR)
- Low energy (< 20 eV) extension : Single-Centre Expansion and R-Matrix procedures

Atoms



Electrons: $V(r) = V_{st}(r) + V_{ex}(r) + V_{pol}(r) + i[V_{abs}(r)]$

Positrons: $V(r) = V_{st}(r) + V_{pol}(r) + i[V_{abs}(r) + V_{ps}(r)]$

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Molecules

Differential cross sections

$$\frac{d\sigma^{elastic}_{molecule}}{d\Omega} = \sum_{i,j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} = \sum_i |f_i(\theta)|^2 + \sum_{i \neq j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}}$$

Integral cross sections

$$\sigma^{total}_{molecule} = \sum_{atoms} \sigma^{total}_{atomi} + \sigma^{interference}$$

$$\sigma^{interference} \equiv \int d\Omega \sum_{i \neq j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}}$$

Calculations

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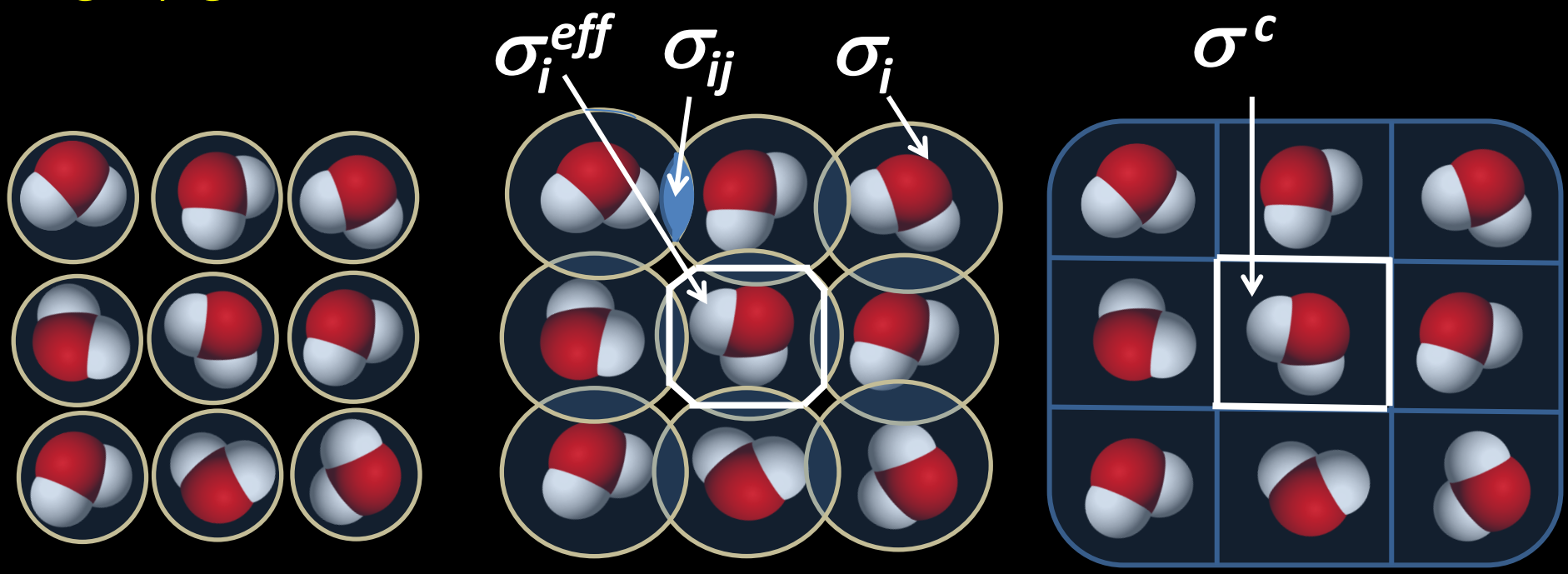
Condensed matter

$\sigma \rightarrow \sigma^{eff}$



High → Intermediate → Low Energy

Corrective factor: $s=\sigma^{eff}/\sigma=[1+(\sigma^c/\sigma)^p]^{1/p}$

P=-21→0,5% convergence

Calculations

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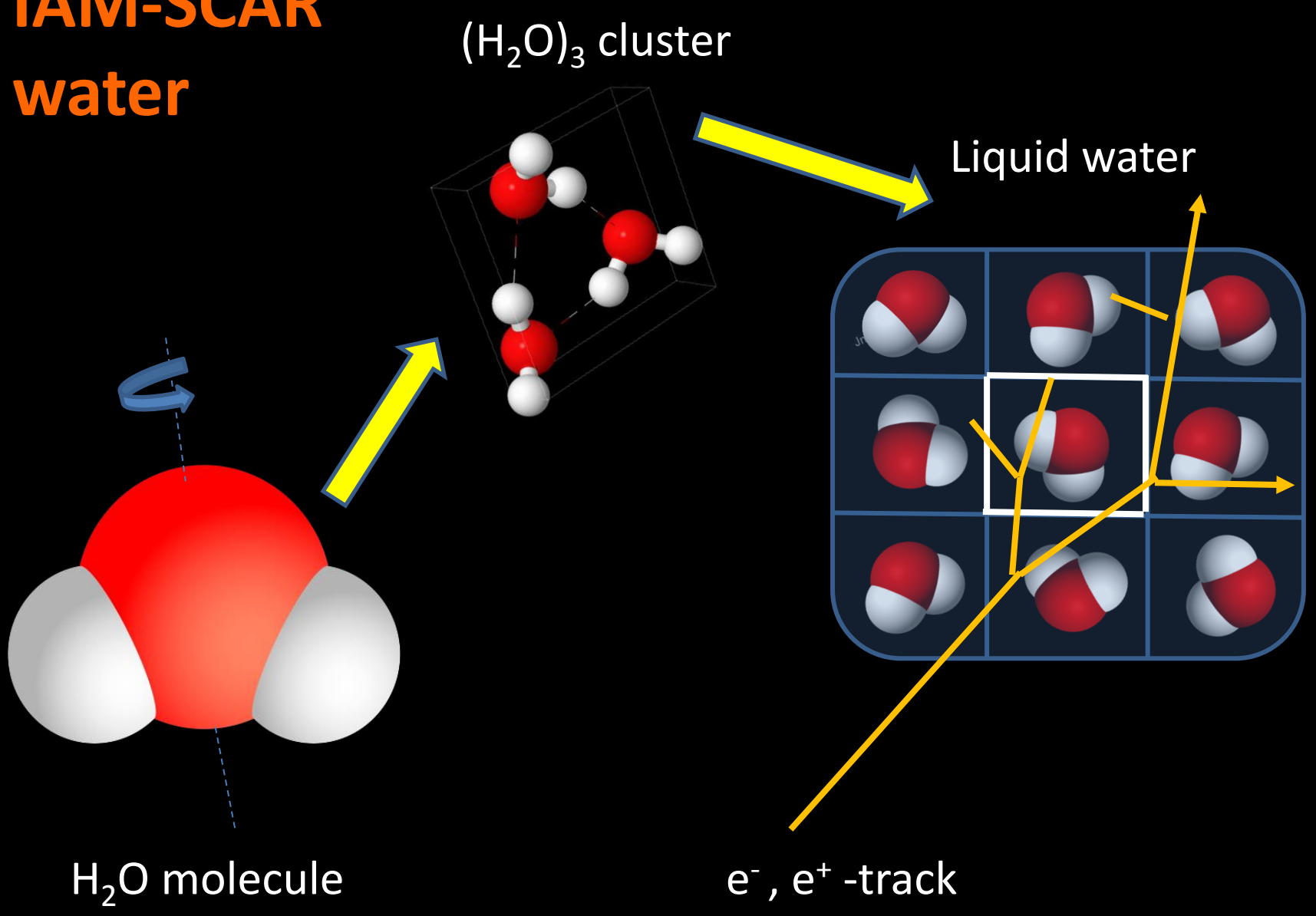
IAM-SCAR water

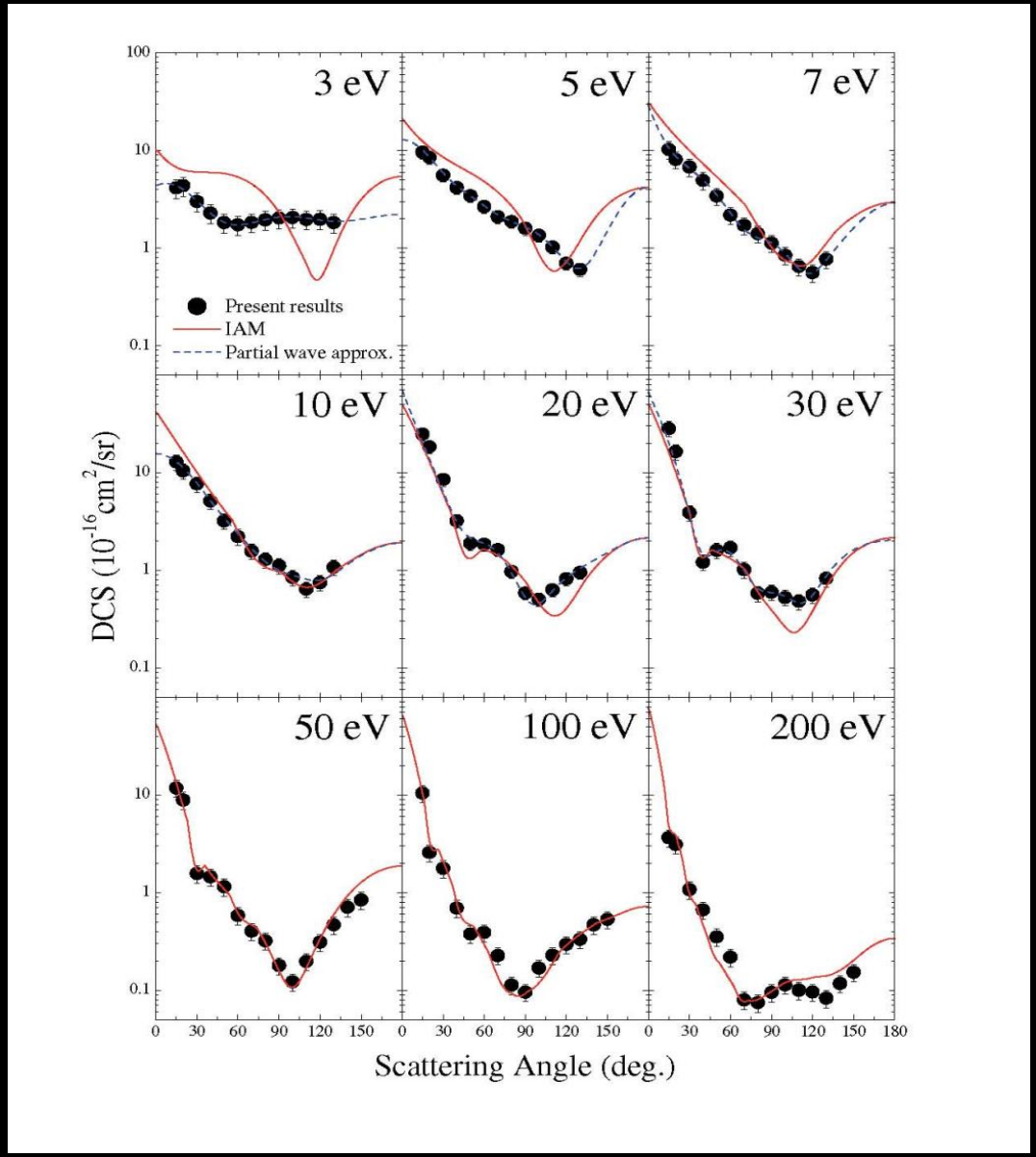


Some examples of calculations

Differential elastic scattering cross sections e-GeF_4

- Experimental data from **H. Tanaka** (SU Tokyo)

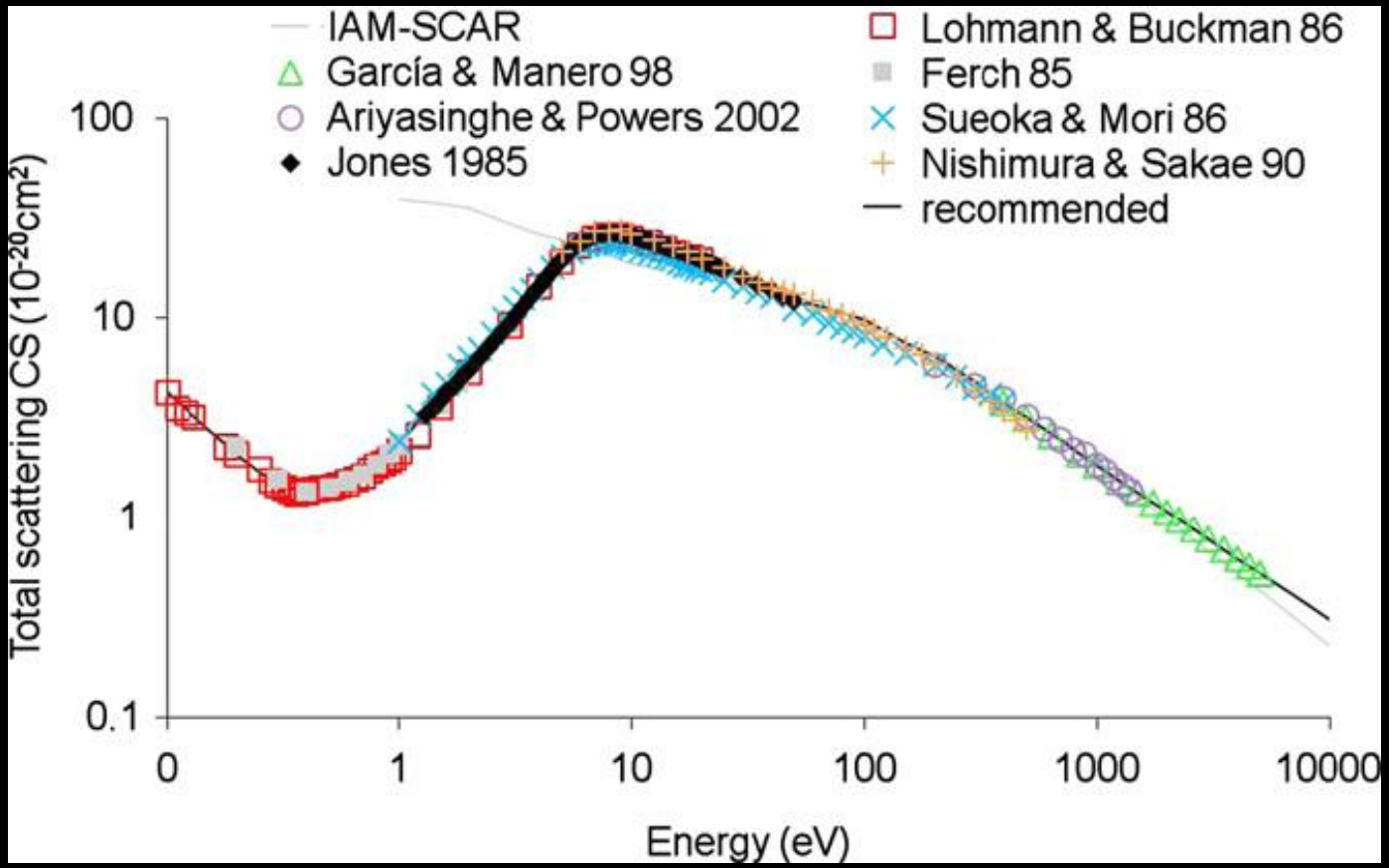
— **IAM-SCAR** calculation



Some examples of calculations

Total electron scattering cross sections

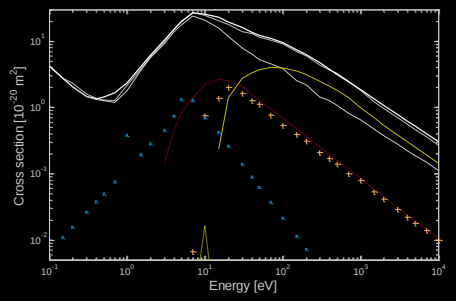
e-CH_4

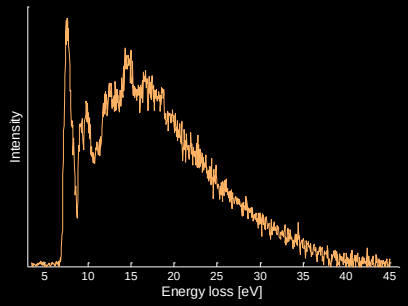


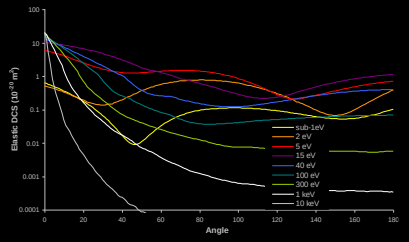
Example of input data

Three main classes of input data are needed:

1. Scattering CS	2. Energy loss distrib. functions	3. Angular distrib. functions







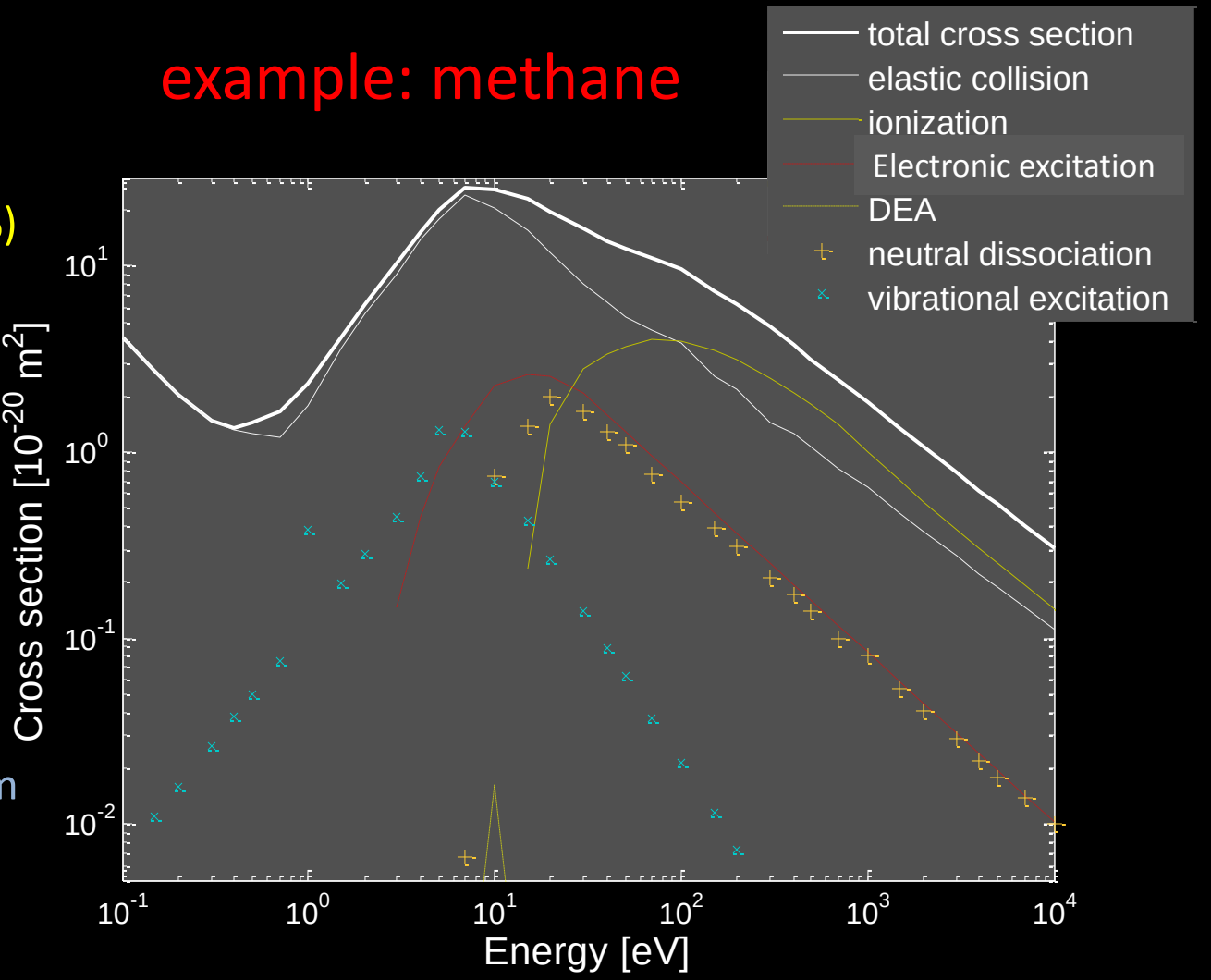
Uncertainties: 5-20% 10-20% 10-20%

Integral CS: 0.1 eV – 10 keV

1. Scattering CS

- Total scattering CS (5-7%)
- Integral CS for:
  - elastic scattering (10-15%)
  - Ionization (7-10%)
  - electronic excitation (20%)
  - vibrational excit. (20%)
  - rotational excit. (10-15%)
  - neutral dissociation (25%)
  - DEA (10-15%)
  - self-consistency:
    Σ int. CS = total CS
- CS table is compiled from typically ~ 15 different sources!

example: methane

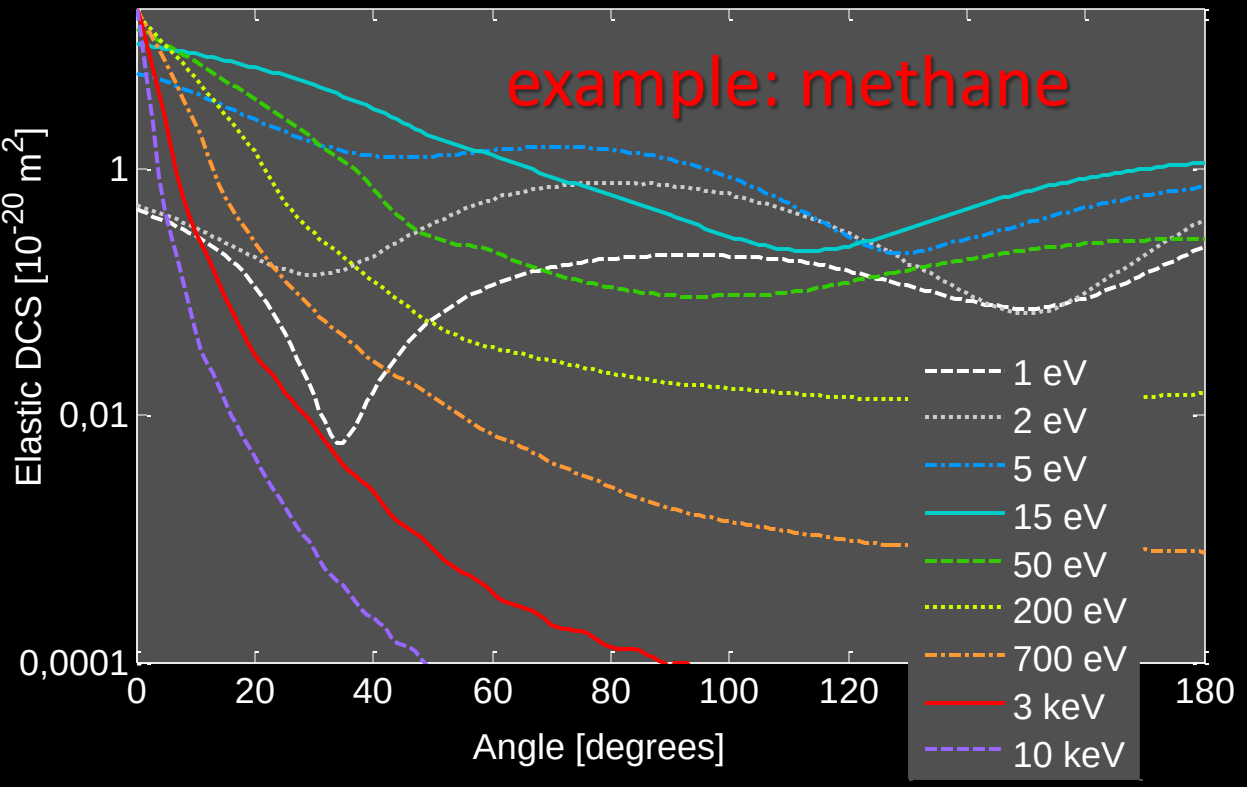


Differential CS 0° -180°

3. Angular distrib. functions

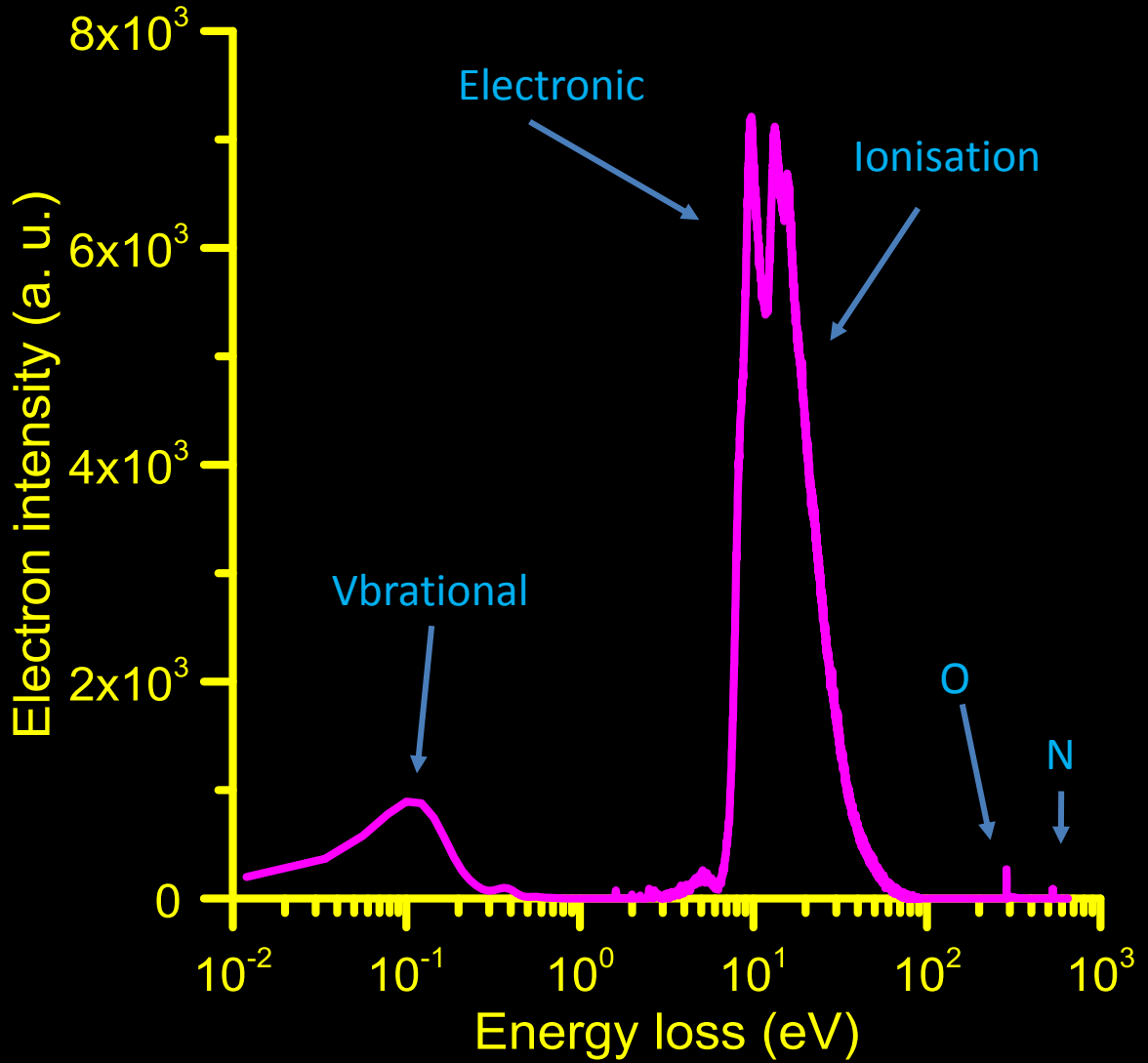
- Elastic DCS
  - Tabulated values from 0° to 180° on a 1° grid from ~6 sources
  - Data from experimental sources are extrapolated towards 0° and 180°
- Inelastic DCS
  - Aim: tabulated form, 0°-180°
  - present source: approximation by empirical formula

$$\frac{\mathrm{d}^2\sigma(E)}{\mathrm{d}\Omega\,\mathrm{d}\Delta E} \propto \left(\frac{\mathrm{d}\sigma(E)}{\mathrm{d}\Omega}\right)_{el}^{1-\Delta E/E}$$



e-Furfural

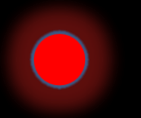
Energy loss distribution function



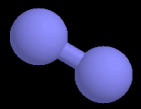
Current state of the Madrid data collection

Molecules currently included:

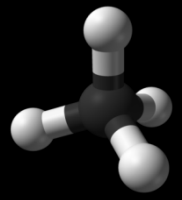
- Water (e, p)



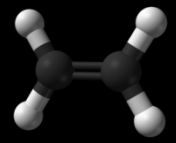
- Argon (e,p)



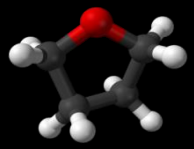
- Nitrogen, Oxygen (e,p)



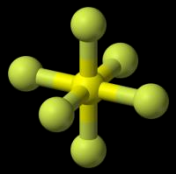
- Methane (e)



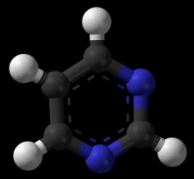
- Ethylene (e)



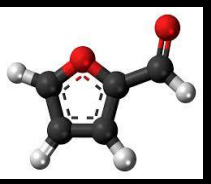
- Tetrahydrofuran (e)



- Sulphur hexafluoride (e)



- Pyrimidine (e, p)

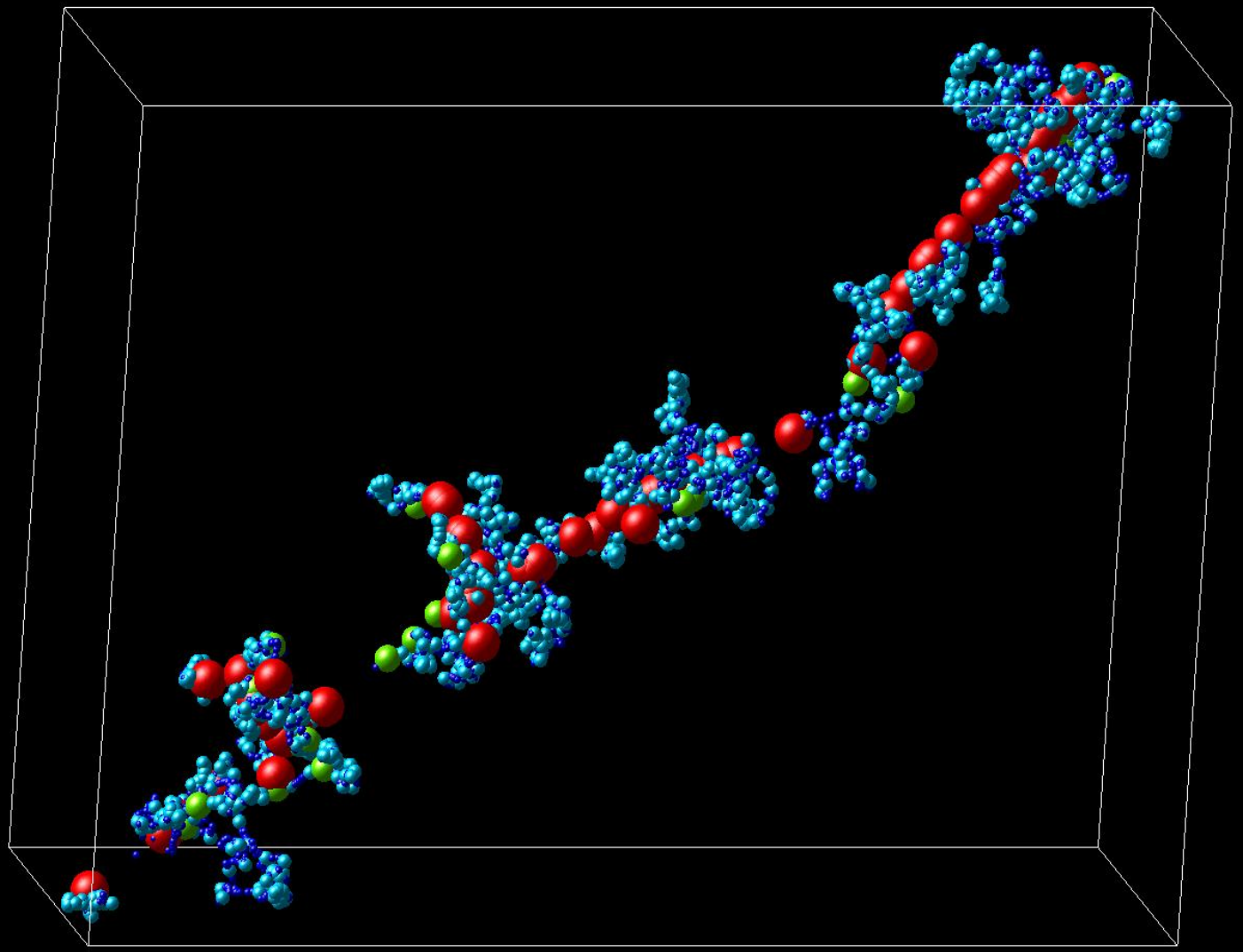


- Furfural (e)

Processes currently included:

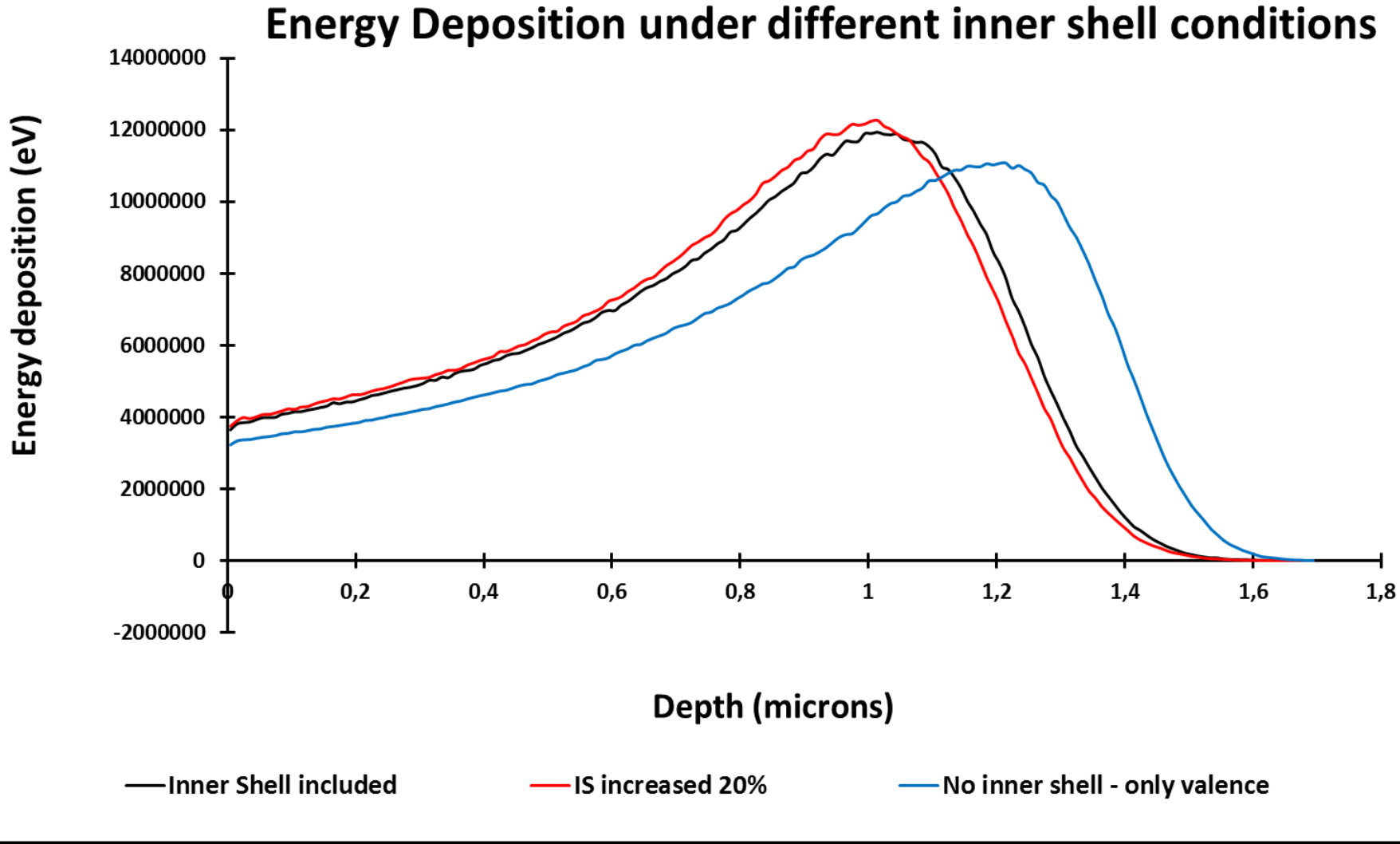
- elastic scattering
- ionization, Auger e- generation
- vibrational and rotational excitation (average of existing states)
- electronic excitation (all states according to EEL spectra)
- neutral dissociation
- dissociative electron attachment
- positronium formation
- annihilation

Example: 10keV electrons through furfural

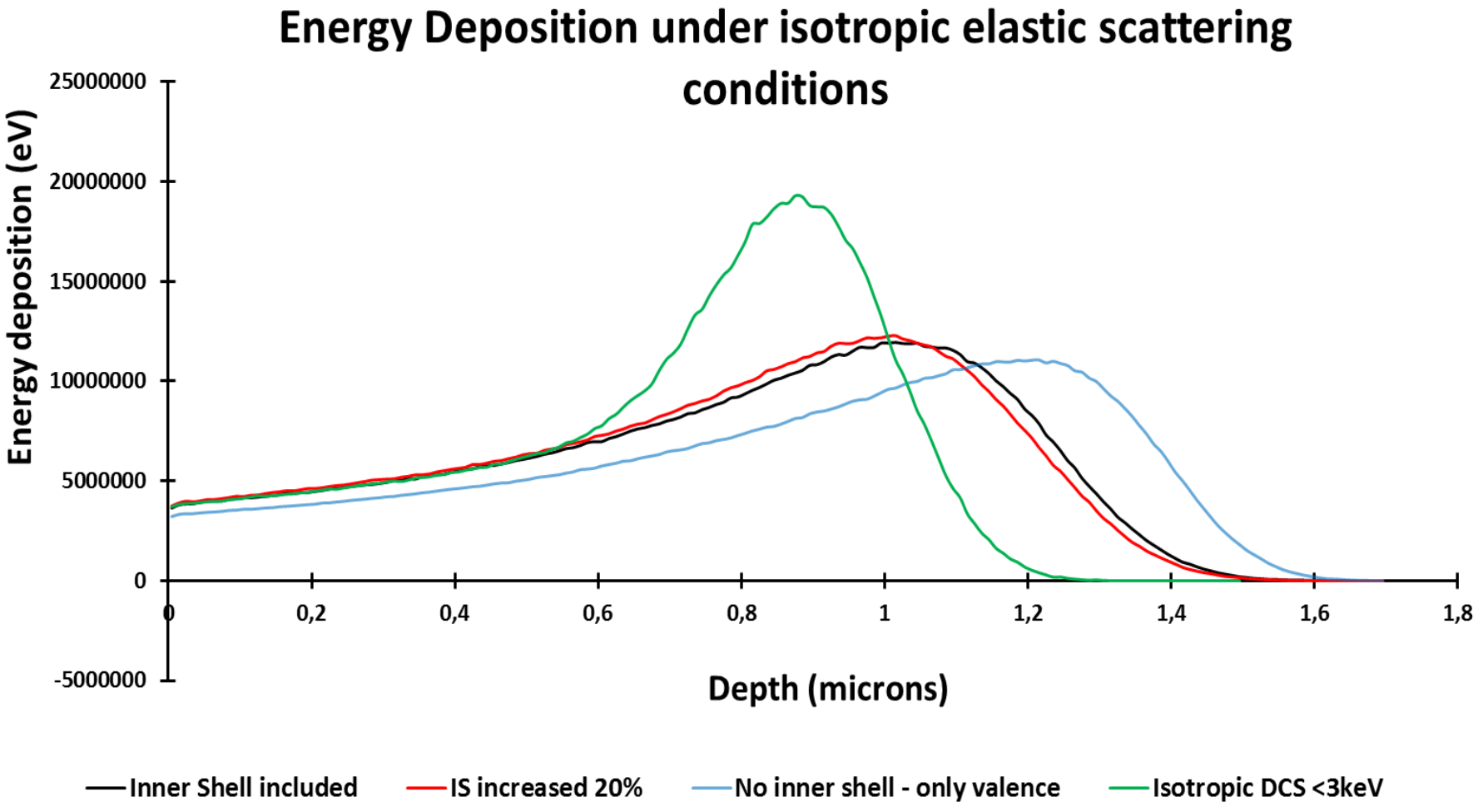


Plot - i2 Interaction type
Density: 1,16013 g/cm3
Mass: 4,39778e-27 g
Edep: 1710,89 eV
2,74114e-16 Joule
Dose: 6,23302e+10 Gy
width: 25,4203 nm
height: 19,0214 nm
depth: 7,83976 nm

Importance of energy loss uncertainties

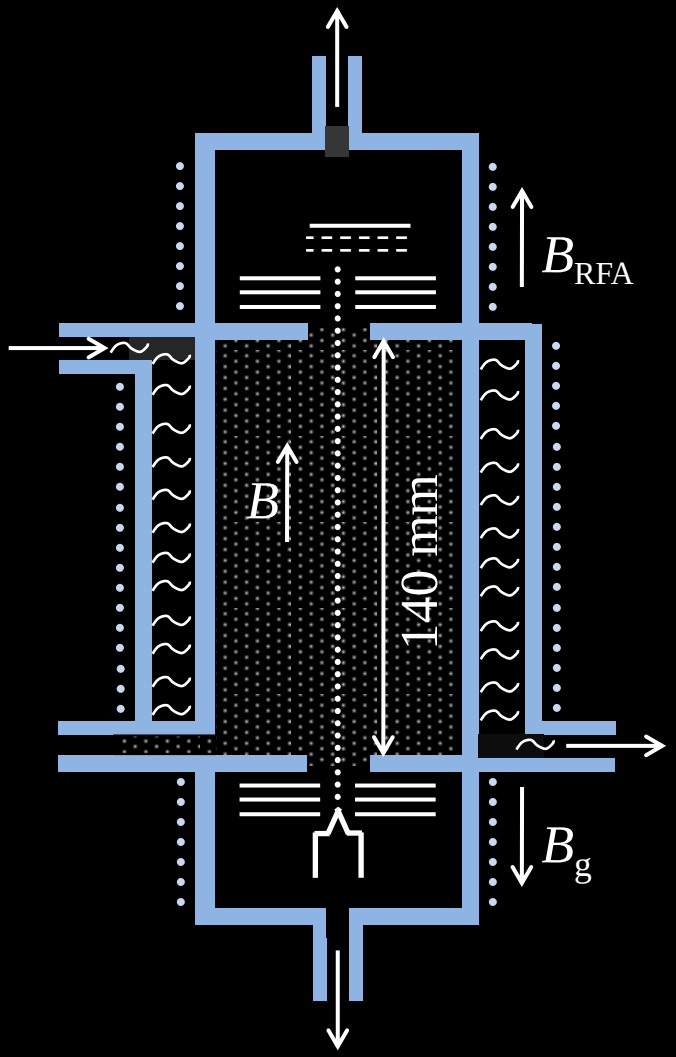


Importance of elastic scattering



Particle transport data evaluation:

20 eV magnetically confined electrons transmitted through 140 mm length gas (3 mTorr furfural pressure) cell



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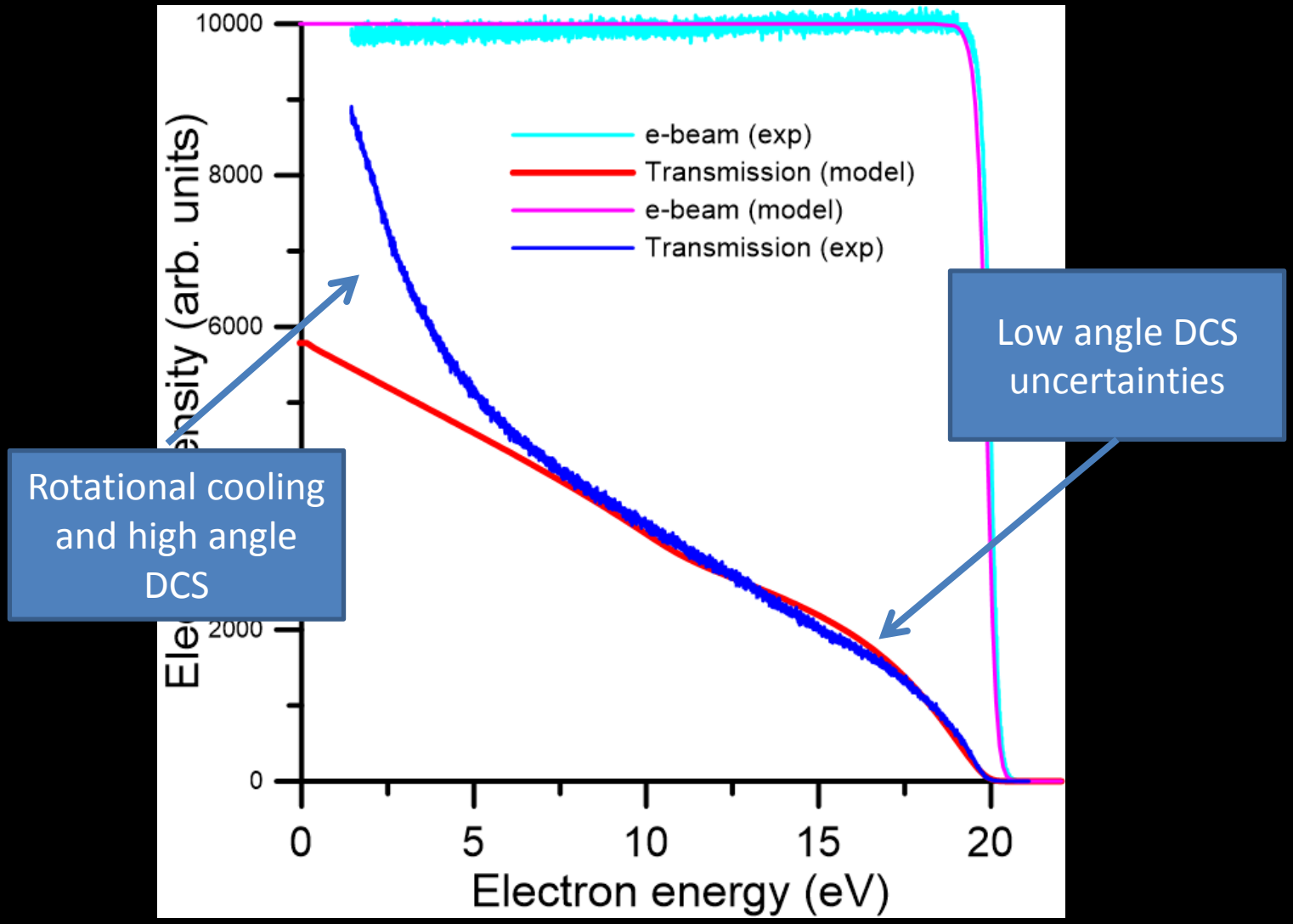

Acknowledgements

- Madrid Group: F. Blanco, A. Muñoz, L. Ellis-Gibbings
- Lisbon (UNL): P. Limão-Vieira, F. Ferreira
- Flinders University (Adelaide): M. Brunger
- ANU (Canberra): S. Buckman, R. McEachran
- J. Cook University (Townsville): R. White
- IOP (Belgrade): B. Marinkovic, Z. Petrovic
- Open University (UK): J. Gorfinkiel
- Innsbruck University: F. Gianturco
- Sherbrooke University: L. Sanche